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# Characterization of graphs having extremal Randić indices<sup>☆</sup>

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## Abstract

The higher Randić index  $R_t(G)$  of a simple graph  $G$  is defined as

$$R_t(G) = \sum_{i_1 i_2 \dots i_{t+1}} \frac{1}{\sqrt{\delta_{i_1} \delta_{i_2} \dots \delta_{i_{t+1}}}},$$

where  $\delta_i$  denotes the degree of the vertex  $i$  and  $i_1 i_2 \dots i_{t+1}$  runs over all paths of length  $t$  in  $G$ . In [J.A. Rodríguez, A spectral approach to the Randić index, *Linear Algebra Appl.* 400 (2005) 339–344], the lower and upper bound on  $R_1(G)$  was determined in terms of a kind of Laplacian spectra, and the lower and upper bound on  $R_2(G)$  were done in terms of kinds of adjacency and Laplacian spectra. In this paper we characterize the graphs which achieve the upper or lower bounds of  $R_1(G)$  and  $R_2(G)$ , respectively.

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## 1. Introduction

Let  $G = (V, E)$  be a simple, connected and finite graph with vertex set  $V = \{1, 2, \dots, n\}$  and edge set  $E$ . Let  $\delta_i$  be the degree of the vertex  $i$  for  $i = 1, 2, \dots, n$ . The minimum degree of a graph is denoted by  $\delta$  and the maximum by  $\Delta$ . The *neighborhood* of a vertex  $i \in V$ , denoted by  $N_i$ , is the set of vertices adjacent to  $i$ . Let  $|X|$  denote the cardinality of a finite set  $X$ .

The *Randić index* or *connectivity index*,  $R_1(G)$ , of a graph  $G$  was introduced by the chemist Milan Randić in 1975 [9] as

$$R_1(G) = \sum_{ij} \frac{1}{\sqrt{\delta_i \delta_j}},$$

where  $ij$  runs over all edges in  $G$ .

The *higher Randić index* or *higher connectivity index* is also of interest in molecular graph theory. For  $t \geq 1$ , the *higher Randić index* is defined by

$$R_t(G) = \sum_{i_1 i_2 \dots i_{t+1}} \frac{1}{\sqrt{\delta_{i_1} \delta_{i_2} \dots \delta_{i_{t+1}}}},$$

where  $i_1 i_2 \dots i_{t+1}$  runs over all paths (that is,  $i_1 i_2, i_2 i_3, \dots, i_t i_{t+1}$  are edges of  $G$  and the  $i_j$  are distinct but possibly  $i_1 = i_{t+1}$ ) of length  $t$  in  $G$ .

Now we define the *weighted adjacency matrix* and the *weighted Laplacian matrix* of a graph [10]. The *weighted adjacency matrix* [10] of a graph  $G$  of order  $n$  is the  $n \times n$  matrix  $A(G)$  whose  $(i, j)$ -entry is

$$a_{ij} = \begin{cases} \frac{1}{\sqrt{\delta_i \delta_j}} & \text{if } ij \in E, \\ 0 & \text{otherwise.} \end{cases}$$

Denote the *weighted adjacency spectrum* of  $G$  by

$$\text{Spec}(A) = \{\lambda_1^{m'_1}, \dots, \lambda_d^{m'_d}\},$$

where  $\lambda_1 < \dots < \lambda_d$  are the eigenvalues of  $A(G)$  and  $m'_i$  is the multiplicity of  $\lambda_i$ .

The *weighted Laplacian matrix* [10] of  $G$  is the  $n \times n$  matrix  $L(G) = (\ell_{ij})_{n \times n}$ , where

$$\ell_{ij} = \begin{cases} \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} & \text{if } i = j, \\ -\frac{1}{\sqrt{\delta_i \delta_j}} & \text{if } ij \in E, \\ 0 & \text{otherwise.} \end{cases}$$

Clearly,  $L(G)$  is a real symmetric matrix. From this fact and Geršgorin's theorem, it follows that its eigenvalues are non-negative real numbers. Moreover since the row sum is 0, the smallest eigenvalue is  $\mu_0 = 0$  with corresponding eigenvector  $\mathbf{j} = (1, 1, \dots, 1)$ . Since  $G$  is assumed to be connected,  $\mu_0$  is an eigenvalue of multiplicity one. Denote the *weighted Laplacian spectrum* of  $G$  by

$$\text{Spec}(L) = \{\mu_0^1, \mu_1^{m_1}, \dots, \mu_b^{m_b}\},$$

where  $0 = \mu_0 < \mu_1 < \dots < \mu_b$  are the eigenvalues of  $L(G)$  and  $m_i$  is the multiplicity of  $\mu_i$ .

The Randić index has been successfully related to physical and chemical properties of organic molecules and becomes one of the most popular molecular descriptors. So it is significant and necessary to investigate the relations between the graph-theoretic properties of  $G$  and its weighted

adjacency or Laplacian eigenvalues. Bounds and characterization of graphs for the largest adjacency or Laplacian eigenvalue, and Laplacian spectrum for unweighted graphs have been investigated to a great extent in the literature [4–7] and references there in. Initially, the Randić index was studied only by chemists, but recently it has also attracted the attention of mathematicians, for instance, see [1,2,3,8]. Rodríguez [10] introduced a suitable version of the adjacency and Laplacian matrix of a graph and has established bounds on  $R_1(G)$  and  $R_2(G)$  in terms of the graph spectra respectively. In this paper we characterize the graphs which achieve the upper and lower bounds of  $R_1(G)$  and  $R_2(G)$ , respectively.

## 2. Bound on Randić index and characterization of graphs

**Lemma 2.1** [12]. Let  $A$  be a  $p \times p$  symmetric matrix and let  $A_k$  be its leading  $k \times k$  submatrix; that is,  $A_k$  is the matrix obtained from  $A$  by deleting its last  $p - k$  rows and columns. Then, for  $i = 1, 2, \dots, k$ ,

$$\lambda_{p-i+1}(A) \leq \lambda_{k-i+1}(A_k) \leq \lambda_{k-i+1}(A), \quad (1)$$

where  $\lambda_i(A)$  is the  $i$ th largest eigenvalue of  $A$ .

**Theorem 2.2.** Let  $G$  be a connected graph. Then

$$\mu_b \geq \frac{1}{2} \max_{ij \in E} \left\{ \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} + \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} + \sqrt{\left( \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} - \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} \right)^2 + \frac{4}{\delta_i \delta_j}} \right\}, \quad (2)$$

where  $\delta_i$  is the degree of the vertex  $i$ .

**Proof.** Using Lemma 2.1 we have

$$\mu_b \geq \max_{ij \in E} \{\mu_b(L_{ij}(G))\},$$

where  $L_{ij}(G)$  is the  $2 \times 2$  submatrix of  $L(G)$  consisting of the  $(i, i)$ ,  $(i, j)$ ,  $(j, i)$  and  $(j, j)$ -entries.

Now one can show that  $\mu_b(L_{ij}(G))$  satisfies the following equation:

$$|L_{ij}(G) - \mu I_2| = \begin{vmatrix} \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} - \mu & -\frac{1}{\sqrt{\delta_i \delta_j}} \\ -\frac{1}{\sqrt{\delta_i \delta_j}} & \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} - \mu \end{vmatrix} = 0 \quad \text{for any edge } ij \in E,$$

i.e.,

$$\begin{aligned} \mu_b^2(L_{ij}(G)) - \left( \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} + \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} \right) \mu_b(L_{ij}(G)) \\ + \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} - \frac{1}{\delta_i \delta_j} = 0 \quad \text{for any edge } ij \in E, \end{aligned}$$

or equivalently,

$$\mu_b(L_{ij}(G)) = \frac{1}{2} \left\{ \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} + \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} + \sqrt{\left( \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} - \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} \right)^2 + \frac{4}{\delta_i \delta_j}} \right\}.$$

The result follows immediately.  $\square$

**Theorem 2.3.** Let  $G$  be a connected graph. Then

$$\mu_1 \leq \frac{1}{2} \min_{ij \in E} \left\{ \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} + \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} + \sqrt{\left( \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} - \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} \right)^2 + \frac{4}{\delta_i \delta_j}} \right\}, \quad (3)$$

where  $\delta_i$  is the degree of the vertex  $i$ .

**Proof.** Putting  $i = 2$  in (1) we have

$$\mu_1 \leq \min_{ij \in E} \{\mu_b(L_{ij}(G))\},$$

where  $L_{ij}(G)$  is the  $2 \times 2$  submatrix of  $L(G)$  consisting of the  $(i, i)$ ,  $(i, j)$ ,  $(j, i)$  and  $(j, j)$ -entries. Using a technique similar to that in Theorem 2.2 we get the required result.  $\square$

**Corollary 2.4.** Let  $G$  be a connected graph. Then

$$\mu_1 \leq \max_{ij \in E} \left\{ \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} + \frac{1}{\sqrt{\delta_i \delta_j}} \right\}, \quad (4)$$

where  $\delta_i$  is the degree of the vertex  $i$ .

**Proof.** Suppose that (3) gives the minimum at the edge  $ij$ . Without loss of generality, one can assume that

$$\sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} \geq \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}}. \quad (5)$$

From (3), we get

$$\begin{aligned} \mu_1 &\leq \frac{1}{2} \left\{ \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} + \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} + \sqrt{\left( \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} - \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} \right)^2 + \frac{4}{\delta_i \delta_j}} \right\} \\ &\leq \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} + \frac{1}{\sqrt{\delta_i \delta_j}} \quad \text{by (5)} \\ &\leq \max_{ij \in E} \left\{ \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} + \frac{1}{\sqrt{\delta_i \delta_j}} \right\}. \quad \square \end{aligned}$$

**Theorem 2.5.** Let  $G$  be a connected graph of order  $n$ . Then

$$\mu_b \geq \frac{n}{n-1}, \quad (6)$$

with equality if and only if  $G$  is the complete graph  $K_n$ .

**Proof.** First, to show the inequality (6), we choose the highest degree vertex, say 1, of degree  $\Delta$ . Let  $j$  be an adjacent vertex of 1 such that  $\delta_j \geq \delta_k$  for all  $k \in N_1$ . Since  $1j \in E$  and  $\delta_1 = \Delta$ , from (2) we have

$$\mu_b \geq \frac{1}{2} \left\{ \sum_{k \in N_1} \frac{1}{\sqrt{\Delta\delta_k}} + \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j\delta_k}} + \sqrt{\left( \sum_{k \in N_1} \frac{1}{\sqrt{\Delta\delta_k}} - \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j\delta_k}} \right)^2 + \frac{4}{\Delta\delta_j}} \right\}. \quad (7)$$

Three cases arises (i)  $\delta_j = \Delta$ , (ii)  $\delta_j = \Delta - 1$ , or (iii)  $\delta_j \leq \Delta - 2$ .

Case (i):  $\delta_j = \Delta$ . We have

$$\text{either } \sum_{k \in N_1} \frac{1}{\sqrt{\Delta\delta_k}} \geq \sum_{k \in N_j} \frac{1}{\sqrt{\Delta\delta_k}} \quad \text{or} \quad \sum_{k \in N_1} \frac{1}{\sqrt{\Delta\delta_k}} < \sum_{k \in N_j} \frac{1}{\sqrt{\Delta\delta_k}}.$$

Without loss of generality, we assume that

$$\sum_{k \in N_1} \frac{1}{\sqrt{\Delta\delta_k}} \geq \sum_{k \in N_j} \frac{1}{\sqrt{\Delta\delta_k}}. \quad (8)$$

By ignoring the term  $\left( \sum_{k \in N_1} \frac{1}{\sqrt{\Delta\delta_k}} - \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j\delta_k}} \right)^2$  in (7), we get

$$\begin{aligned} \mu_b &\geq \frac{1}{2} \left\{ \sum_{k \in N_1} \frac{1}{\sqrt{\Delta\delta_k}} + \sum_{k \in N_j} \frac{1}{\sqrt{\Delta\delta_k}} + \frac{2}{\Delta} \right\} \quad \text{as } \delta_j = \Delta \\ &\geq \sum_{k \in N_j} \frac{1}{\sqrt{\Delta\delta_k}} + \frac{1}{\Delta} \quad \text{by (8)}. \end{aligned} \quad (9)$$

Now,

$$\begin{aligned} \sum_{k \in N_j} \frac{1}{\sqrt{\Delta\delta_k}} + \frac{1}{\Delta} - \frac{n}{n-1} &= \frac{1}{\Delta} \sum_{k \in N_j} \frac{\sqrt{\Delta} - \sqrt{\delta_k}}{\sqrt{\delta_k}} + \frac{n-1-\Delta}{(n-1)\Delta} \\ &\geq 0, \quad \text{because } \Delta \geq \delta_k \text{ for all } k; \text{ and } n-1 \geq \Delta. \end{aligned} \quad (10)$$

Using (9), we have

$$\mu_b \geq \frac{n}{n-1}.$$

Case (ii):  $\delta_j = \Delta - 1$ . By ignoring the term  $\left( \sum_{k \in N_1} \frac{1}{\sqrt{\Delta\delta_k}} - \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j\delta_k}} \right)^2$  in (7), we get

$$\begin{aligned} \mu_b &\geq \frac{1}{2} \left\{ \sum_{k \in N_1} \frac{1}{\sqrt{\Delta\delta_k}} + \sum_{k \in N_j} \frac{1}{\sqrt{(\Delta-1)\delta_k}} + \frac{2}{\sqrt{\Delta(\Delta-1)}} \right\} \\ &\geq \frac{1}{2} \left\{ \sqrt{\frac{\Delta}{\Delta-1}} + \sqrt{\frac{\Delta-1}{\Delta}} + \frac{2}{\sqrt{\Delta(\Delta-1)}} \right\} \\ &= \frac{\Delta + \frac{1}{2}}{\sqrt{\Delta(\Delta-1)}}. \end{aligned} \quad (11)$$

Now,

$$\begin{aligned} \frac{\left(\Delta + \frac{1}{2}\right)^2}{\Delta(\Delta - 1)} - \frac{n^2}{(n - 1)^2} &= \frac{1}{\Delta(\Delta - 1)(n - 1)^2} \left( \left(\Delta + \frac{1}{2}\right)^2 (n - 1)^2 - n^2(\Delta^2 - \Delta) \right) \\ &= \frac{1}{\Delta(\Delta - 1)(n - 1)^2} \left( 2n\Delta(n - \Delta - 1) + \Delta^2 + \Delta + \frac{1}{4}(n - 1)^2 \right) \\ &> 0. \end{aligned}$$

Using (11) we have

$$\mu_b > \frac{n}{n - 1}.$$

Case (iii):  $\delta_j \leq \Delta - 2$ . By ignoring the term  $\frac{4}{\Delta\delta_j}$  in (7), we get

$$\mu_b > \sum_{k \in N_1} \frac{1}{\sqrt{\Delta\delta_k}} \geq \sqrt{\frac{\Delta}{\Delta - 2}}. \quad (12)$$

Now,

$$\begin{aligned} \frac{\Delta}{\Delta - 2} - \left(\frac{n}{n - 1}\right)^2 &= \frac{1}{(\Delta - 2)(n - 1)^2} \left( (n - 1)^2 \Delta - n^2(\Delta - 2) \right) \\ &= \frac{1}{(\Delta - 2)(n - 1)^2} (2n(n - \Delta) + \Delta) > 0. \end{aligned}$$

Using (12) we have

$$\mu_b > \frac{n}{n - 1}.$$

Now suppose that the equality holds in (6). Then we can see easily that the graphs can be characterized from Case (i) only, because in the other two cases inequalities are strict. Then all inequalities in the Case (i) must be equalities and also the equality holds in (7). From the equality in (10), we get

$$\delta_k = \Delta \quad \text{for all } k \in N_j \text{ and } \Delta = n - 1. \quad (13)$$

In Case (i) we have  $\delta_j = \Delta$ . Thus, by (13), we have  $\delta_j = n - 1$  and  $\delta_k = n - 1$  for all  $k \in N_j$ . Hence  $G$  is the complete graph  $K_n$ . Also the equality holds in (7) for the complete graph  $K_n$ .

Conversely, one can see easily that the equality holds in (6) for the complete graph  $K_n$ .  $\square$

**Lemma 2.6** [2,11]. *Let  $G$  be a connected graph of order  $n$ . Then*

$$R_1(G) \leq \frac{n}{2}. \quad (14)$$

Using Lemma 2.6 and Theorem 2.5 we get the following theorem.

**Theorem 2.7.** *Let  $G$  be a connected graph of order  $n$ . Then  $\mu_1 = \mu_2 = \cdots = \mu_b$  if and only if  $G$  is the complete graph  $K_n$ .*

**Proof.** If  $G$  is the complete graph of order  $n$ , then  $\mu_1 = \mu_2 = \cdots = \mu_b = \frac{n}{n-1}$  holds.

Conversely, when  $\mu_1 = \mu_2 = \cdots = \mu_b$ , we need to show that  $G$  is the complete graph  $K_n$ . Suppose that  $G$  is not the complete graph of order  $n$ . Using Theorem 2.5 one can conclude that

$$\mu_b > \frac{n}{n-1}. \quad (15)$$

Thus,

$$\mu_1 = \mu_2 = \cdots = \mu_b > \frac{n}{n-1}.$$

It was shown in [10] that

$$\begin{aligned} R_1(G) &= \frac{1}{2} \sum_{i=1}^b m_i \mu_i \\ &> \frac{1}{2} (n-1) \frac{n}{n-1} \text{ by (15),} \end{aligned}$$

that is,  $R_1(G) > \frac{n}{2}$ . It contradicts to Lemma 2.6. Hence  $G$  should be the complete graph  $K_n$ .  $\square$

Rodríguez [10] has established the following relation but not characterized the graphs when the equality holds. For completeness we include a short proof of this result.

**Theorem 2.8.** *Let  $G$  be a connected graph. Then the Randić index of  $G$  is bounded by*

$$\frac{(n-1)\mu_1}{2} \leq R_1(G) \leq \frac{(n-1)\mu_b}{2}. \quad (16)$$

*Moreover, the equality holds for either side if and only if  $G$  is the complete graph  $K_n$ .*

**Proof.** We have

$$2R_1(G) = \text{Tr}(L(G)) = \sum_{i=1}^b m_i \mu_i.$$

From this we can get the required result.

The necessary and sufficient condition for the equalities in both sides is that all the non-zero Laplacian eigenvalues are equal. Using Theorem 2.7 we conclude that the equalities on both sides in (16) hold if and only if  $G$  is the complete graph  $K_n$ .  $\square$

**Lemma 2.9** (Rayleigh-Ritz [13]). *If  $A$  is a symmetric  $n \times n$  matrix with eigenvalues  $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$  then for any  $\mathbf{u} \in \mathbb{R}^n$  ( $\mathbf{u} \neq \mathbf{0}$ ),*

$$\mathbf{u}^T A \mathbf{u} \leq \rho_1 \mathbf{u}^T \mathbf{u}. \quad (17)$$

*Equality holds if and only if  $\mathbf{u}$  is an eigenvector of  $A$  corresponding to the largest eigenvalue  $\rho_1$ .*

Rodríguez [10] has established another relation in Theorem 2.10 but did not find the condition for which the equality holds. For completeness we sketch the proof of this relation.

**Theorem 2.10.** *Let  $G = (V, E)$  be a connected bipartite graph with bipartition  $V = (X; Z)$ . Then the Randić index of  $G$  is bounded by*

$$R_1(G) \leq \frac{|X||Z|}{|X| + |Z|} \mu_b, \quad (18)$$

where  $\mu_b$  is the largest eigenvalue of  $L(G)$ . Moreover, the equality holds if and only if  $\sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}}$  is independent of the choice of  $i \in X$  or of  $i \in Z$ .

**Proof.** Let  $X = \{1, 2, \dots, k\}$  and  $Z = \{k+1, k+2, \dots, k+\ell = n\}$ . Also let  $\mathbf{u} = (u_1, u_2, \dots, u_n)$  be the vector defined by

$$u_i = \begin{cases} r & \text{if } i \in X, \\ -s & \text{if } i \in Z \end{cases}$$

such that  $kr = \ell s$ . So,  $r = \frac{r+s}{k+\ell} \ell$  and  $s = \frac{r+s}{k+\ell} k$ . Thus,  $kr^2 + \ell s^2 = \frac{k\ell}{k+\ell} (r+s)^2$ . Using (17), we have

$$\mathbf{u}^T L(G) \mathbf{u} \leq \mu_b \mathbf{u}^T \mathbf{u},$$

i.e.,

$$\left( \sum_{i \in N_1} \frac{1}{\sqrt{\delta_1 \delta_i}} r + \sum_{i \in N_1} \frac{1}{\sqrt{\delta_1 \delta_i}} s, \dots, \sum_{i \in N_k} \frac{1}{\sqrt{\delta_k \delta_i}} r + \sum_{i \in N_k} \frac{1}{\sqrt{\delta_k \delta_i}} s, - \sum_{i \in N_{k+1}} \frac{1}{\sqrt{\delta_{k+1} \delta_i}} r \right. \\ \left. - \sum_{i \in N_{k+1}} \frac{1}{\sqrt{\delta_{k+1} \delta_i}} s, \dots, - \sum_{i \in N_n} \frac{1}{\sqrt{\delta_n \delta_i}} r - \sum_{i \in N_n} \frac{1}{\sqrt{\delta_n \delta_i}} s \right) \mathbf{u} \leq \mu_b (kr^2 + \ell s^2),$$

i.e.,

$$r^2 \sum_{ij} \frac{1}{\sqrt{\delta_i \delta_j}} + s^2 \sum_{ij} \frac{1}{\sqrt{\delta_i \delta_j}} + 2rs \sum_{ij} \frac{1}{\sqrt{\delta_i \delta_j}} \leq \mu_b (kr^2 + \ell s^2),$$

i.e.,

$$\mu_b \geq \frac{(r+s)^2}{kr^2 + \ell s^2} R_1(G), \text{ because } R_1(G) = \sum_{ij} \frac{1}{\sqrt{\delta_i \delta_j}},$$

i.e.,

$$\mu_b \geq \frac{|X| + |Z|}{|X||Z|} R_1(G), \text{ because } kr^2 + \ell s^2 = \frac{k\ell}{k+\ell} (r+s)^2. \quad (19)$$

This completes the proof of (18).

Now suppose that the equality holds in (18). Then all inequalities in the above argument must be equalities. Using Lemma 2.9 we conclude that  $\mathbf{u}$  is an eigenvector corresponding to the largest Laplacian eigenvalue  $\mu_b$  of  $L(G)$ . From  $L(G)\mathbf{u} = \mu_b \mathbf{u}$ , we have for  $i \in X$ ,

$$\mu_b r = \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} r + s \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}},$$

i.e.,

$$\mu_b = \frac{r+s}{r} \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}}. \quad (20)$$

Similarly, from  $L(G)\mathbf{u} = \mu_b \mathbf{u}$ , we have for  $i \in Z$ ,

$$\mu_b = \frac{r+s}{s} \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}}. \quad (21)$$

Thus,  $\sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}}$  is independent of  $i \in X$  or  $i \in Z$ .



Conversely, let  $\sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}}$  be independent of  $i \in X$  or  $i \in Z$ . Since  $G$  is a bipartite graph with bipartition  $X$  and  $Z$ , we get

$$|X| \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} = |Z| \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} \quad \text{for } i \in X \text{ and } j \in Z \quad (22)$$

and

$$R_1(G) = |X| \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} = |Z| \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} \quad \text{for } i \in X \text{ and } j \in Z. \quad (23)$$

We need to show that  $R_1(G) = \frac{|X||Z|}{|X|+|Z|} \mu_b$ . To do this, let  $\mu_b$  be the largest Laplacian eigenvalue corresponding to an eigenvector  $\mathbf{y} = (y_1, y_2, \dots, y_n)^T$  of  $L(G)$ . One can assume that one of the eigencomponents, say  $y_i$  is equal to 1 and the other eigencomponents are less than or equal to 1 in magnitude, that is,  $y_i = 1$  and  $|y_k| \leq 1$  for all  $k$ . Also let  $|y_j| = \max\{|y_k| : k \in N_i\}$ . From the  $i$ th row of  $L(G)\mathbf{y} = \mu_b \mathbf{y}$ , we have

$$\mu_b y_i = \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} y_i - \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} y_k,$$

i.e.,

$$\mu_b \leq \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} (1 + |y_j|) \quad \text{as } |y_j| \geq |y_k| \text{ for all } k, k \in N_i. \quad (24)$$

From the  $j$ th row of  $L(G)\mathbf{y} = \mu_b \mathbf{y}$ , we have

$$\mu_b y_j = \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} y_j - \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} y_k,$$

i.e.,

$$\mu_b |y_j| \leq \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} (1 + |y_j|), \quad \text{because } |y_k| \leq 1 \text{ for all } k. \quad (25)$$

From (24) and (25) we get

$$\mu_b (1 + |y_j|) \leq \left( \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} + \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} \right) (1 + |y_j|),$$

i.e.,

$$\begin{aligned} \mu_b &\leq \left( \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} + \sum_{k \in N_j} \frac{1}{\sqrt{\delta_j \delta_k}} \right) \\ &= \frac{|X| + |Z|}{|Z|} \sum_{k \in N_i} \frac{1}{\sqrt{\delta_i \delta_k}} \quad \text{by (22)} \\ &= \frac{|X| + |Z|}{|X||Z|} R_1(G) \quad \text{by (23)}. \end{aligned} \quad (26)$$

From (19) and (26), we get

$$\mu_b = \frac{|X| + |Z|}{|X||Z|} R_1(G).$$

Hence the theorem is proved.  $\square$

### 3. Bound on higher Randić index and characterization of graphs

Rodríguez [10] established the following relation in Theorem 3.1 but not characterized the graphs when the equality holds. For a completeness we include a short proof of this result.

**Theorem 3.1.** *Let  $G$  be a connected graph. Let*

$$\text{Spec}(A) = \{\lambda_1^{m'_1}, \dots, \lambda_d^{m'_d}\} \quad \text{and} \quad \text{Spec}(L) = \{\mu_0^1, \mu_1^{m_1}, \dots, \mu_b^{m_b}\}$$

*be the weighted adjacency spectrum and the weighted Laplacian spectrum of  $G$ , respectively. Then the second Randić index of  $G$ ,  $R_2(G)$ , is bounded as*

$$\frac{\sqrt{\delta}}{2} \left( \sum_{i=1}^b m_i \mu_i^2 - 2 \sum_{i=1}^d m'_i \lambda_i^2 \right) \leq R_2(G) \leq \frac{\sqrt{\Delta}}{2} \left( \sum_{i=1}^b m_i \mu_i^2 - 2 \sum_{i=1}^d m'_i \lambda_i^2 \right). \quad (27)$$

*Moreover, the equality holds on the right side in (27) if and only if  $G$  is a regular graph or  $G$  is only two type of degrees  $\Delta$  and one; while the equality holds on the left side in (27) if and only if  $G$  is a regular graph.*

**Proof.** We have

$$\begin{aligned} \text{Tr}(L^2) &= 4 \sum_{ij \in E} \frac{1}{\delta_i \delta_j} + 2 \sum_{ijk} \frac{1}{\sqrt{\delta_j \delta_i \delta_j \delta_k}} \\ &= 2\text{Tr}(A^2) + 2 \sum_{ijk} \frac{1}{\sqrt{\delta_j \delta_i \delta_j \delta_k}}. \end{aligned} \quad (28)$$

Thus,

$$\frac{2}{\sqrt{\Delta}} R_2(G) \leq \text{Tr}(L^2) - 2\text{Tr}(A^2) \leq \frac{2}{\sqrt{\delta}} R_2(G). \quad (29)$$

Hence, the result follows.

Next, we suppose that the equality holds on the right side in (27). Then the equality holds on the left side in (29). From (28) and equality on the left side in (29), we get  $\delta_j = \Delta$  for each path  $ijk$ . Since  $G$  is connected,  $\delta_j = \Delta$  for all non-pendant vertices. If  $G$  contains a pendant vertex then  $G$  has only two types of degrees  $\Delta$  and one, otherwise  $G$  is a regular graph. Similarly, we can show that  $G$  is a regular graph if the equality holds on the left side in (27).

Conversely, we can see easily that the equality holds on the right side in (27) for the graphs which have only two types of degrees  $\Delta$  and one, or are regular graphs, while the equality holds on the left side in (27) for regular graphs.  $\square$

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